 | **ITST**
INSTITUTE FOR TERAHERTZ
SCIENCE AND TECHNOLOGY

Annual Report
UCSB 2010-2011

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Mission Statement

The mission of ITST is to advance science and technology at the heart of the electromagnetic spectrum* while training and inspiring new generations of scientists, engineers, and the public at large and supporting research with outstanding service in a warm, welcoming and fun workplace.



Figure 1: Chart showing ITST's research emphasis at the heart of the electromagnetic spectrum.

3 *roughly 0.1-10 terahertz (1 terahertz= 10^{12} cycles/s). For reference, cell phones transmit near 1 GHz (10^9 cycles/s) and the spectrum of visible light stretches from about 400-800 terahertz.

Director's Statement

The field of terahertz science and technology is experiencing explosive growth. Over the last decade, the number of publications in the field has increased more than six-fold, from 400 to 2600.¹ This year has seen the launch of a new high-quality journal of the IEEE entitled “Terahertz Science and Technology.”

The increasing breadth and impact of terahertz science and technology was beautifully represented at the 2011 international Workshop on Optical Terahertz Science and Technology (OTST 2011), which was hosted by ITST in March 2011.² The workshop was a resounding success, with over 200 attendees from 19 countries, including 67 students. The photograph on the cover of this report shows a poster session from the workshop. Talks and posters covered a wide range of topics, including art conservation; the diffusion of oxygen through Portuguese cork; the complex molecular dance of proteins with water;³ and the discovery, using terahertz spectroscopy of the perforated electron gas⁴. Roughly half of the conference participants joined a tour of UCSB, including ITST's Free-Electron Lasers and other powerful spectrometers that have been recently commissioned. While UC Santa Barbara has long been recognized as a world-leading center for terahertz science and technology, the OTST workshop increased ITST's international visibility.

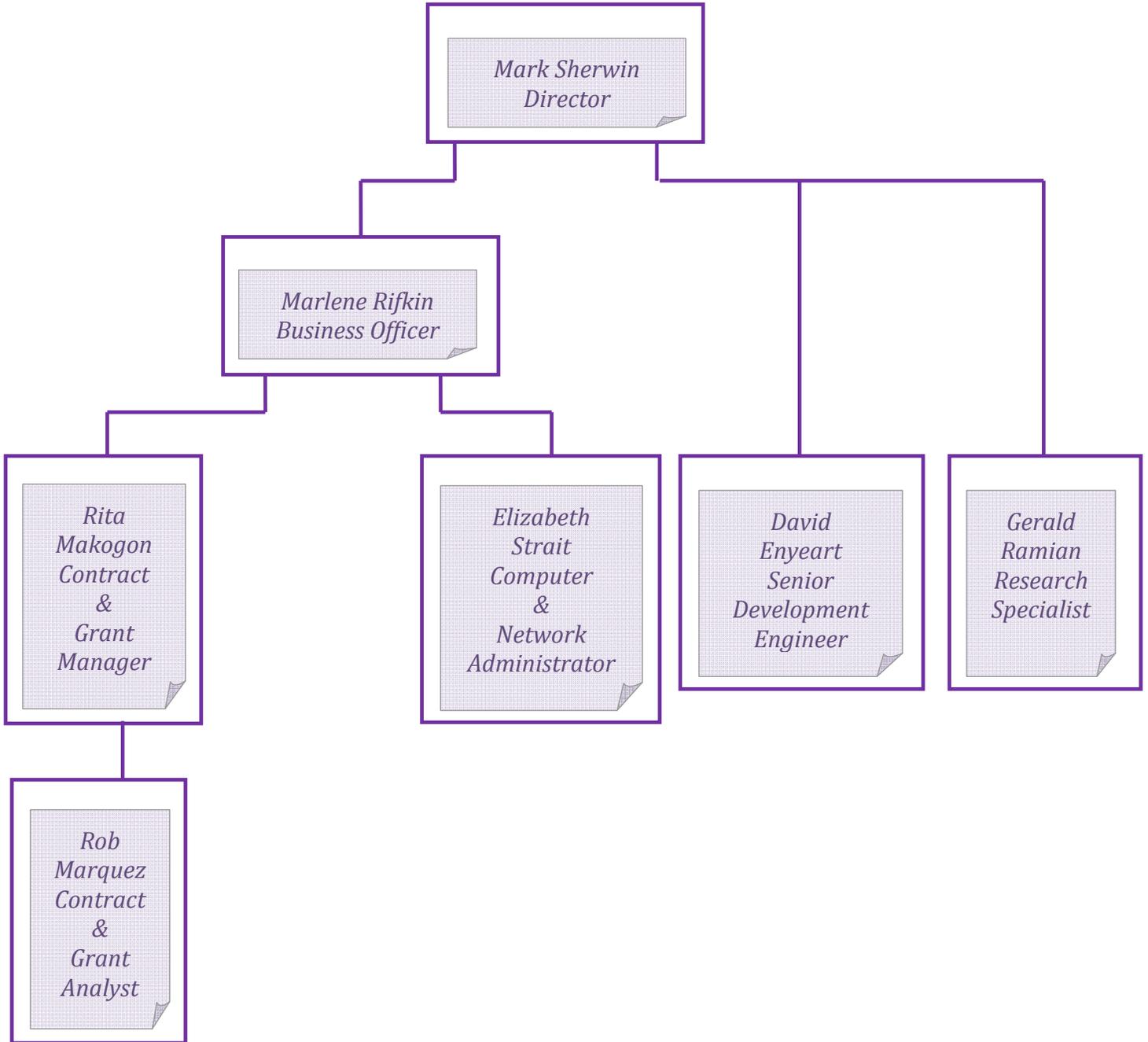
The visibility and impact of ITST on campus is continuously growing through our Thursday seminar series⁵ --now held in our new home, building 937, just West of Broida Hall. An increasing number of investigators are taking advantage of our unique and state-of-the art terahertz instrumentation.

ORU's at UCSB have dual functions—to serve as centers for interdisciplinary research, and to excel in the pre- and post-award administration of contracts and grants. A core mission of ITST is —“supporting research with outstanding service in a warm, welcoming and fun workplace.” ITST is UC Santa Barbara's only ORU focused in the physical sciences. As you will see if you glance through the summaries of the exciting research projects we administer, we continue to welcome and serve principal investigators from a wide range of departments in the sciences and engineering, regardless of the intellectual focus of their research. We are particularly proud of long-time PI Prof. Bruce Lipshutz, who this year won the Presidential Green Challenge Chemistry Award for discoveries enabling important chemical reactions to proceed in water, without toxic organic solvents.

We are looking forward to continuing to grow the community of terahertz researchers at UC Santa Barbara and elsewhere, while providing outstanding administrative support for contract and grant administration for researchers in all areas of science and engineering.

1. Numbers from Web of Science search with Topic=terahertz.
2. Many many thanks to Marlene Rifkin and Elizabeth Strait for making this a great success!
3. A research highlight from ITST, graphic shown in the “sky” above the poster session (N. Q. Vinh, K. W. Plaxco and S. J. Allen, *Journal of the American Chemical Society* 2011)
4. Another ITST research highlight, C. M. Morris et. al., *NanoLetters* 2011. In the artist's landscape below the photo on the cover, the electron gas is represented as a colorful “sea,” with orange corresponding to the deepest “water” (most electrons). A high density of electrons trapped in the volcanic “craters” (which represent cylindrical nanostructures developed at UCSB) is shown in red. What look like volcanic islands rise above the electrons that make up the sea, which is repelled by the electrons in the crater. For scale, the craters are about 30 nanometers in diameter.
5. Please see the attractive poster on p. 8.

Organizational Chart



Advisory Committee

Songi Han	Chemistry and Biochemistry, Committee Chair
S. James Allen	Former iQuest Director, Physics
Ben Mazin	Physics
Christopher Palmstrom	Electrical and Computer Engineering
Kevin Plaxco	Chemistry and Biochemistry
Susanne Stemmer	Materials Department
Win Van Dam	Computer Science

Ex Officio Members

Omer Blaes	Chair, Physics
Rick Dahlquist	Chair, Chemistry and Biochemistry
Marlene Rifkin	Business Officer, ITST
Mark Sherwin	Director, ITST, Physics

Personnel

Administrative Staff-ITST

Marlene Rifkin, Business Officer
Rita Makogon Contract and Grant Manager
Rob Marquez Contract and Grant Analyst
Elizabeth Strait Computer and Network Administrator

Technical Staff-ITST

David Enyeart Senior Development Engineer
Gerald Ramian Research Specialist

Other Project and Activities

OTST 2011

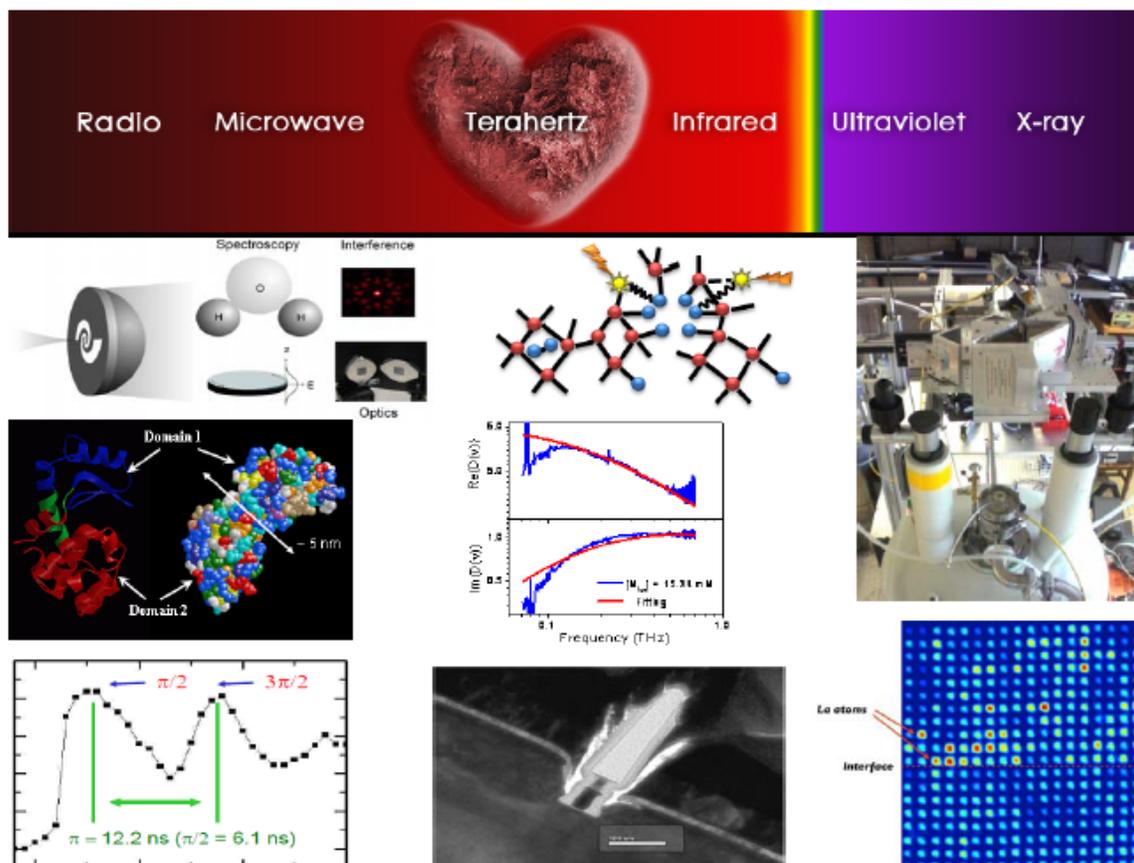
March 13, 2011– March 17, 2011
Fess Parker Doubletree Hotel, Santa Barbara



In March, 2011, ITST successfully hosted the International Workshop on Optical Terahertz Science and Technology, 2011 (OTST 2011). The aim of the workshop was to foster discussion on the newest and most exciting research in the development and applications of terahertz instrumentation based on optical sources. Over 200 people, including 67 students, from 19 countries attended the conference.

Seminars and Workshops

ITST continued its very successful lunchtime Seminar Series. Refreshments (usually pizza) were provided. The following seminars took place throughout the year:



10/07/10:

Terahertz Spectroscopy Comes of Age: Dr. Mark Sherwin, ITST and Physics Department, University of California, Santa Barbara

10/14/10:

Pulsed EPR (ESR) in the THz Frequency Range and Nanosecond Time Scale: Dr. LC Brunel, ITST, University of California, Santa Barbara

10/21/10:

A Broadly Tunable THz Source Based on Photomixing in “n-i-pn-i-p” Superlattices: Dr. Sascha Preu, ITST and Materials Department, University of California, Santa Barbara

10/25/10:

Watch Water Dancing with Protein: Hydration Dynamics and Coupled Water-Protein Fluctuations: Prof. Dongping Zhong, Ohio State University

10/28/10:

Probing the Dynamics of Biomolecules in Liquid Water By Terahertz Spectroscopy: Dr. Vinh Nguyen, ITST, University of California, Santa Barbara

11/04/10:

A Superconducting Spectrophotometer for the Palomar and Keck Telescopes: Dr. Benjamin Mazin, Physics Department, University of California, Santa Barbara

12/02/10:

High-Mobility Complex Oxide Heterostructures by MBE : Dr. Susanne Stemmer, Materials Department, University of California, Santa Barbara

02/03/11:

Viscosity of Electrolytes: Dr. Fyl Pincus, Physics and Materials Departments, University of California, Santa Barbara

02/17/11:

Design of THz Field Effect Transistors: Dr. Mark Rodwell, Electrical and Computer Engineering Department, University of California, Santa Barbara

03/10/11:

Shallow Donors in Silicon Serving as Electron and Nuclear Spin Qubits: Dr. J. van Tol, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida

03/31/11:

Nanometer Range Distance Measurements in Biomolecules by High Field Pulse EPR using Gd³⁺ Spin Labels: Dr. Daniella Goldfarb, The Weizmann Institute of Science, Rehovot, Israel

04/07/11:

Electron Spin-Amplified Nuclear Magnetic Resonance at High Fields: Dr. Songi Han, ITST and Chemistry and Biochemistry Department, University of California, Santa Barbara

04/18/11:

Optimal Control of Spins: Robust Pulses and Decoupling: Prof. Steffen Glaser, TU Munich, Germany

04/28/11:

Tuning in on the Frequencies of the Hydrogen Bond Network of Water: Dr. Matthias Heyden, Chemistry Department, University of California, Irvine

Awards Administered

(July 2010 – June 2011)

NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

Guenter Ahlers

National Science Foundation, DMR-0702111

Turbulent Convection in a Fluid Heater from Below

05/01/07-04/30/12

\$775,000

Turbulent convection in a fluid heated from below occurs naturally in Earth's atmosphere and oceans where it influences climate and weather, in Earth's mantle where it contributes to the motion of continental plates, in Earth's outer core where it determines the magnetic field, in the Sun where it influences the temperature on Earth, and in many industrial processes where it may have significant economic consequences. This grant supports experiments under highly controlled laboratory conditions and in samples of idealized shapes where some of the central physical components of this process can be studied quantitatively. These components include relatively quiet fluid layers just above the bottom and below the top plate (the "boundary layers"), and a turbulent interior with highly fluctuating temperature and fluid-flow. A large convection cell, known as the "wind of turbulence", is superimposed on these interior fluctuations. Quantitative measurements will be made of the turbulent enhancement of the heat transport, of the temperature distribution in the interior, and of the wind dynamics. The highly quantitative experiments are of modest complexity and thus afford an exceptional diverse learning experience for both graduate and undergraduate students who participate in the work.

Dirk Bouwmeester

National Science Foundation, PHY-0804177

Quantum States of OptoMechanical Structures

08/01/08-07/31/12

\$600,000

Quantum theory has been extremely successful in explaining many aspects of the world around us. Despite this achievement, fundamental aspects of the quantum theory are as mysterious as they were to the founders of the theory. Especially remarkable is the feature that a particle somehow obtains information about different "paths" it could have taken. This observation leads to the question of what would happen if such quantum effects could be observed in macroscopic objects. If the laws of quantum mechanics remain valid for large objects, one seems to be forced to accept that cats can be alive and dead at the same time (following Schroedinger's famous thought experiment). However, others question

whether such a drastic conclusion is justified based on the current support for the theory. The fact is that all experiments to date that directly tested the quantum superposition of individual objects are restricted to photons, atoms, molecules and ensemble of electrons. Furthermore the quantum theory is faced with problems when trying to unify it with the theory of relativity. It is not possible either on theoretical or experimental grounds, therefore, to rule out the possibility that quantum mechanics does not apply to large objects. Optical technology has progressed to the level that it is conceivable to put a small mirror into a superposition of two quantum states. The experiment will be done with a particularly tiny mirror, smaller in diameter than a human hair but still about ten billion times more massive than any object previously brought into a quantum superposition. This award provides support for the mirror and cantilever fabrication as well as for designing a liquid-helium cooled apparatus and performing supporting theoretical work. Furthermore it provides travel support for establishing a close collaboration with international experts on sub-millikelvin systems. Testing quantum mechanics in this unexplored regime is first of all of fundamental importance. The optical control of micro-mechanical systems, in particular the application of optical cooling techniques, is however also expected to be of broad interest in metrology and could also be used for several different experiments such as generating squeezed light and resonance enhanced Casimir forces. This research program involves significant educational component, and the research is excellent for teaching fundamental properties of quantum mechanics and micro-mechanical systems and for training young researchers in state-of-the-art technologies in a multi-disciplinary and international environment.

Dirk Bouwmeester
Pierre Petroff
National Science Foundation, ECCS-0901886
Solid State Cavity Electrodynamics
06/03/09-08/31/12
\$399,914

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

The objective is to develop solid-state devices for achieving controlled and efficient coupling between single photons and single electrons confined in microstructures.

Dirk Bouwmeester
Elisabeth Gwinn
Deborah Fygenon
Everett Lipman
Michael Liebling
National Science Foundation, DMR-0960331
MRI-R2 Nano Photonic Imaging System
03/15/10-2/28/13
\$464,703

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

A rapidly expanding field of research concerns the development of new techniques for optical imaging of nanometer to micron scale structures, such as biological molecules with integrated functional elements, semiconductor optoelectronic devices and cells. The investigator team proposes to develop an unconventional optical instrument capable of resolving structures on the scale of a few tens of nanometers, by using special correlated states of light (such as entangled two-photon states) in combination with an ultra stable optical platform with nanometer resolution scanning capabilities and recently-developed signal processing algorithms. In order to probe the special light-matter interactions that occur when phonon-induced dephasing is minimal, the system is designed to operate at cryogenic as well as ambient temperatures. The wide wavelength range of this nano-photonics imaging system would enable investigation of structures ranging from semiconductor nanodevices to DNA scaffolds to living cells. The research team consists of experts in the key technological aspects: quantum optics, high resolution optical imaging and high speed image processing, ultra-low vibration and low-temperature operation, and biological system design.

Michael Bowers
Air Force, FA9550-06-1-0069
POSS and Metal Clusters: Structures and Energetics
01/01/06-05/31/11
\$936,000

There are several objectives for this proposal:

1. Structure and Characterization of Polyhedral Oligomeric Silsesquioxane (POSS) attached to Polymer Backbones: The POSS family of molecules has recently generated great interest due to their inherent thermal and chemical stability and their ability to improve the thermal, physical and chemical properties of host polymer systems. We have developed ion-mobility-based mass spectrometric methods suitable for characterizing a wide variety of POSS cages. In the coming three years, these methods, coupled with

extensive molecular modeling will be applied to POSS cages covalently bound to oligomers of a variety of organic polymers. We will collaborate with a number of synthetic research groups in the development of rational synthetic strategies to produce these materials.

2. Size-Selected Structures and Ligand Binding Energies of Metal Clusters: In recent years there has been a major renaissance in the study of small metal clusters as catalytic agents for select, important industrial processes. Of special importance are the clusters of coinage metals: gold, silver and (possibly) copper. At UCSB we have constructed a unique instrument for the deposition and characterization of size-selected coinage metal clusters on metal oxide surfaces, funded by a multi-investigator DURINT grant. There are several aspects of this work that are strongly complemented by gas phase studies, Careful STM measurements have established that clusters of four or more gold atoms have specific structures on the surface and that the onset of the transition from 2-dimensional to 3-dimensional surface clusters occurs below $n=8$. It will be very important to know the actual structures of the species that are deposited at low energies onto the surfaces to see if they correlate with observed surface structures. Theory also plays a large role in interpreting the structure and reactivity of surface-deposited systems. Careful measurement of structures and ligand binding energies of size- and charge-selected gas-phase clusters is crucial for providing experimental benchmarks for testing theoretical models. Finally, shape and ligand binding energy studies over large cluster size ranges allows direct observation of atomic to bulk transitions, an area where much is speculated but little is known.

Michael Bowers

UC Los Angeles, SB070075

Pathogenic Protein Folding and Human Disease

09/01/06-07/31/11

\$1,292,132

The objective of this research is to understand, on a molecular level, the folding and assembly of A β -protein alloforms. Recent results indicate small, soluble oligomers of A β are responsible for initiating a pathological cascade resulting in Alzheimer's disease (AD). A β 42 has been shown to be the primary neurotoxic agent even though A β 40 is nearly 10 times more abundant. Single-point amino-acid substitutions at positions 22 and 23 in A β 42 account for a variety of familial forms of AD. It is our hypothesis that A β monomers and small oligomers are important therapeutic targets and characterization of their structure and mechanisms of folding and assembly are critical research objectives. Here we propose to apply, for the first time, the powerful methods of ion mobility spectrometry coupled with mass spectrometry (IMS-MS) to the problem of A β folding and assembly. These methods provide accurate measures of monomer and oligomer cross sections and oligomer size distributions. When coupled with high-level molecular dynamics modeling, monomeric structure with atomic detail is obtained. The method is ultrasensitive, routinely working with picomoles of sample or less. These methods can be readily extended to other neurological diseases like ALS and Parkinson's disease that share the misfolding/aggregation motif with AD.

The specific aims of this research are (1) to structurally characterize A β monomers and to determine how these structures change with single-amino-acid substitution, oxidation or other simple sequence modification, (2) to structurally characterize A β monomer fragments and determine how these structures change with sequence length, single-amino-acid substitutions or other modifications, and (3) to measure

oligomer-size distributions and oligomer structures for the early stages of assembly of A β and modified forms of A β 40 and A β 42.

Michael Bowers
National Science Foundation, CHE-0909743
Non-Covalent Complexes
08/01/09-07/31/13
\$730,000

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

In this award funded by the Experimental Physical Chemistry Program of the Division of Chemistry, Professor Michael Bowers of University of California, Santa Barbara, explores the question of why peptides and proteins in living systems are solely composed of L-amino acids - one of the deepest mysteries in biology. Professor Bowers and his students will start with several simple model systems of peptides that are available in a wide range of chirally mixed forms. These peptides are small enough (5 or 6 amino acids long) that good theory can be done on them to help understand observed changes in their folding and aggregation tendencies as a function of their chiral purity. These peptide families will also provide an entrée into a second major thrust of the proposal - amyloid formation mechanisms. Amyloids are ubiquitous in complex living systems and are implicated in many serious diseases (Alzheimer's, type 2 diabetes, etc.). The goal is to understand the aggregation process and how initially coiled or alpha-helical oligomeric systems end up as large beta-sheet assemblies. As part of this effort Professor Bower's team will initiate a collaboration with Gerhard Meijer and Gert Von Helden at the Fritz Haber Institute in Berlin. This group is building a state of the art instrument to Professor Bower's specifications for this work to couple with a new free electron laser under construction at that facility. Finally the researchers have initiated studies on a related biologically important amyloid system, the 37 residue IAPP or amylin peptide, involved in type 2 diabetes. The human wild type peptide rapidly forms large oligomers but a number of very similar peptides do not. Preliminary data implicate compact assemblies as leading to fibril formation (and hence disease) while elongated assemblies of the same oligomer number do not aggregate further. Modeling and further experiments are planned to fully understand these initial results.

Science education in the United States is in a sustained downturn that threatens our world leadership in both innovation and technology development. The problems start early. The 5th grade has been targeted as the first "go" or "no go" indicator in a child's scientific development. At UCSB there is a strong outreach program at the 5th grade level initiated and sustained by a former group member with continuing help from current research group members. Professor Bowers decided to tackle the second "go" or "no go" decision time in young adults - their high school years. His group is developing an outreach program using all group members to present their research projects to high school classes and to relate their personal scientific stories and how they ended up in graduate school at UCSB. A

preliminary trial with one of the group members has been run with encouraging results. Additional UCSB faculty and research groups will be incorporated as the program grows.

Michael Bowers

Air Force FA9550-11-1-0113

Litigated Metal Clusters: Structures, Energetics and Reactivity

06/15/11-06/14/14

\$190,000 (\$570,000)

The field of metal clusters, their reactivity and ligand binding energies has undergone a renaissance in recent years. There are two principle drivers: The importance of metal clusters in catalysis and their fundamental importance as bridging agents between the atomic and the solid phases of matter. The Bowers group is uniquely positioned to contribute to this important area of research. They have developed two tools that allow structural determination for size-selected clusters: ion mobility methods that yield accurate cross sections and sequential ligand binding energies that identify equivalent binding sites. These have been applied primarily to coinage metals but here the group will extend these studies to transition metal clusters.

Steven Buratto

Michael Bowers

Department of Energy/Miscellaneous Offices and Programs, DE-FG02-06ER15835

Chemical Imaging with 100nm Spatial Resolution

09/01/06-08/31/10

\$596,299

Over the past decade high resolution optical microscopy methods have been utilized with great success to image the absorbance, luminescence, photoconductivity and Raman scattering of thin films and surfaces with spatial resolution of the order of 100nm. Using conventional far-field optics (i.e. microscope objectives), laser scanning confocal microscopy (LSCM) is capable of probing materials with spatial resolution approaching 200 nm and single molecule sensitivity in fluorescence and surface-enhanced Raman contrast. In addition, a new scanned probe microscopy, near-field scanning optical microscopy (NSOM) method has been developed with the same capabilities and array of applications as

LSCM but with spatial resolution enhanced by nearly an order-of-magnitude. Despite such wide applicability, these imaging methods still lack chemical specificity and often produce images where it is difficult to determine the chemical origin of the image contrast. In order to address this deficiency we

propose to combine, in a single instrument, the high spatial resolution microscopy techniques of LCSM and NSOM with the chemical specificity and conformational selectivity of ion mobility mass spectrometry. We will adapt the source chamber of an ion mobility apparatus to include a combination scanning confocal/near-field microscope. The optical microscopy will be performed in vacuum and an image with luminescence, transmission (absorption) or Raman contrast will be recorded using either the microscope objective or the NSOM optics. In order to determine the chemical contrast from selected domains in the optical image, we will position the sample to the desired spot with the scanning electronics and vaporize molecules from the selected region via laser desorption ionization using the imaging optics. A mass spectrum and/or an arrival time distribution (ATD) will then be recorded from the gas-phase molecules. This data will provide a chemical signature (i.e. mass measurement) and a shape distribution for a given species (ATD) within the localized region of the sample.

Steven Buratto

Michael Bowers

Horia Metiu

National Science Foundation, CHE-0749489

Model Nanocluster Catalysts: The Role of Size, Shape and Composition on the Catalytic Activity on Monometallic, Bimetallic and Metal Oxide Clusters on Oxide Surfaces

04/01/08-03/31/11

\$536,000

In this research supported by the Analytical and Surface Chemistry Program, Professors Buratto, Bowers, and Metiu and their groups will prepare, characterize, and test three new types of nanoscale catalysts, having one feature in common: very small, isolated, well-defined, catalytically active sites. They will prepare and study (a) very small Au_n and Ag_n mass-selected clusters supported on oxide, (b) very small mass-selected, binary clusters such as Pd_mAu_n supported on oxides, and (c) very small, mass-selected oxide clusters supported on oxides. A variety of techniques will be used, in a concerted manner, to study these important catalytic processes: model catalytic systems will be prepared by depositing mass-selected clusters on oxide surfaces to ensure atom-by-atom control of catalyst size; all samples will be prepared and studied in ultra-high vacuum by surface science techniques (AES, XPS) as well as by STM/ AFM before, during and after the catalytic chemistry; and density functional theory (DFT) will be used to calculate the structure of the clusters, their XPS spectrum and their chemical activity. Through the work proposed here they will develop a detailed understanding of the catalytic chemistry of these materials and find out how this chemistry depends on size, composition and the nature of the substrate. While the focus of the research is on the catalytic activity of specific nanoscale catalysts, there is a high probability that the results will be applicable to other systems. In addition, it is hoped that the concepts developed through this research will help optimize important industrial processes using these nanoscale catalysts and provide insight into the discovery of new nanoscale catalytic materials. The research funded by this grant will be interdisciplinary. Graduate students will interact continuously with three different research groups, will have daily contact with other outstanding scientists, and will acquire hands-on experience in a large number of techniques of surface science, gas-

phase chemistry, scanned probe microscopy, and high level theory. The research will provide a valuable opportunity for graduate education, found in very few places in the world. Researchers supported by this grant (including PIs) will also be active in outreach to K-12 schools in the Santa Barbara area to present a tutorial on an atomistic view of heterogeneous catalysis and to show an atomically-resolved picture of our model catalyst systems. This will be included in the currently active outreach program in the chemistry department at UCSB. A series of lectures on catalysis by nanostructures will be developed and included as part of a course in nanoscience currently taught in the materials chemistry curriculum.

David Cannell

National Aeronautics and Space Administration, NNX08AE53G

Gradient Driven Fluctuations

03/01/08-02/28/11

\$190,000

This research continues the work done previously. Although we do not yet have the data in hand, our experiment was flown aboard the Foton-M3 mission on September 14-26, 2007. Hopefully, our results will provide insight into the behavior of single-component fluids and mixtures, including protein solutions, when placed in the microgravity environment, and subjected to temperature and/or concentration gradients. This might be of considerable interest to anyone attempting crystal growth in the microgravity environment, for example, because the growth process of necessity generates concentration gradients, and thus enhanced fluctuations.

Andrew Cleland

National Science Foundation, DMR-0605818

Mechanical Quantum Resonators: Quantum Optics with Phonons

07/01/06-06/30/11

\$355,000

Quantum mechanics controls the behavior of very small, atomic-scale systems like the hydrogen atom and the electron. Demonstrations of the applicability of quantum mechanics to larger scale systems, especially ones with millions or more independent atoms, are challenging due to the need to isolate the system of interest from the environment that surrounds them, an environment that demolishes the quantum effects so peculiar to our classical experience. To date, no clear demonstration of quantum effects in large systems has been performed, certainly not in large mechanical systems. This project will focus on the construction of small mechanical resonators, similar to quartz crystals used to time computer circuits, sufficiently disconnected from the rest of the world to allow quantum effects to be displayed in an unambiguous fashion. In particular, the quantum nature of vibrational energy, which is predicted to change in steps rather than in a continuous fashion, will be explored in detail. The multidisciplinary project integrates research and education in order to train students and postdoctoral

researchers in modern methods required to address this key problem in physics, which will be integrated with engineering and nanotechnology to achieve the goals set forward here. The acquired interdisciplinary skills, which include state-of-the-art nanofabrication and radiofrequency and microwave technology, prepare the trainees for careers in academe, national laboratories, and industry.

Deborah Fygenon

Dirk Bouwmeester

National Science Foundation, CCF-062257

DNA Patterned Pairs of Colloidal Quantum Dots: A Scalable Approach to Computing Without Wires

09/01/06-02/28/11

\$300,000

To reduce the size of computer architecture and test a revolutionary new approach to computation, we will investigate fully self-assembled arrays of classical and quantum bits that are addressed by optical signals only. As bits we propose to use single electron spins in colloidal quantum dots (cqdots). Every cqdot has a specific resonance frequency at which the absorption of a photon can lead to the formation of a trion state (two electrons and one hole confined within a quantum dot). Trion states have large electric dipole moments and can therefore interact over distances of the order of 10 nm. We will leverage the polarization of the illuminating light and the Pauli exclusion principle to control trion formation and subsequently detect the spectral effect of dipole-dipole interactions between cqdots spaced 5 to 10 nm apart. In this manner, we have as a long-term goal the physical realization of theoretical schemes for quantum computing. On the way to this goal, we will explore simplified approaches that are also very interesting from the perspective of classical computation and data storage. For the three-year period of the proposed research, our primary contribution to the quest for all-optical classical and quantum computation will be to address the challenge of nanometer positioning of colloidal quantum dots and to study their optical interactions. Our approach will be to combine self-assembled DNA scaffolds with site-specific binding elements to produce an array of optically active colloidal quantum dots. Self-assembled DNA scaffolds leverage the intrinsic specificity of Watson-Crick base-pairing to organize millions of atoms into close-packed arrays of the familiar double-helical structure with nanoscopic precision. Modern synthesis methods allow decoration of specific atoms in the DNA structure with chemically reactive groups. These reactive groups can be chosen to form covalent links to molecules that stabilize the surface of colloidal quantum dots. By placing the reactive groups at specific sites on the DNA scaffold, pairs of dots and linear or two-dimensional arrays of dots will be patterned, with a spacing that favors quantum mechanical interactions between dots. The resulting structures will be characterized by scanning probe microscopy and the interactions probed by optical pump-probe measurements.

The research will be carried out by a cross-disciplinary research team at the University of California Santa Barbara that is anchored by expertise in self assembly of DNA, the synthesis of colloidal quantum dots and their attachment to functionalized elements at specific locations (Fygenson), and expertise in quantum-optics and solid-state experiments analyzing coupled quantum dots embedded in bulk semiconductor material (Bouwmeester). We will collaborate strongly with Paul W. K. Rothmund, in the Department of Computer Science at Caltech, who recently invented an powerful new class of self-assembling DNA scaffolds that can template arbitrary complex patterns with 6 nm resolution.

Songi Han

Frederick Dahlquist

Mark Sherwin

Louis-Claude Brunel

Johan van Tol

National Science Foundation CHE-0821589

MRI: Development of a 240 Hhz Pulsed Electron Paramagnetic Spectrometer with Nanosecond Time Resolution

08/01/08-07/31/12

\$1,254,623

The Department of Chemistry and Biochemistry at the University of California-Santa Barbara will develop a 240 GHz pulsed electron paramagnetic resonance spectrometer (EPR) with this award from the Major Research Instrumentation (MRI) program. This high frequency EPR spectrometer will capitalize on the tunable terahertz excitation pulses generated at UC Santa Barbara's Free Electron Laser (FEL) facility. The instrument will push the frontier of EPR spectroscopy to more than twice the current frequency/field limitation. It will open up new areas of investigation of the structure and dynamics in biological, chemical and electronic systems.

EPR spectroscopy detects changes in electron spin in materials that contain an unpaired electron. This provides information on the structure and motions of the material at an atomic level. The resultant data provides insight on the properties of materials such as proteins, enzymes and defects in solid materials. This new instrument will allow the study of proteins in biologically relevant environments that were heretofore impossible in many cases. After development, the new spectrometer is intended to become a multi-user facility because of its unique capabilities. Graduate and undergraduate students will be involved in this project learning skills in the design and construction of state-of-the-art instrumentation.

Bruce Lipshutz

UCSB

The Green Initiative Fund (TGIF)

19

NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

Getting Organic Solvents Out of Organic Reactions

06/01/09-06/30/12

\$45,000

Our plan is to devise up to three new experiments that will teach high school and college level students about green chemistry. These will focus on eliminating the major source (i.e. 75+%) of chemical waste: organic solvents. The nanotechnology ("micellar catalysis") in hand and upon which these new experiments are to be based will allow for them to be run in water (actually seawater!) at room temperature; no additional energy consumption/cost should be needed. If realized as envisioned, lab hoods may not even be required. This pilot study may, therefore, be a model that further encourages those who oversee teaching labs in Chemistry to design elements of sustainability (i.e. "benign by design") into their curricula so as to focus on minimizing use of organic solvents.

Bruce Lipshutz

National Institutes of Health, 1R01 GM086485-01A1

New Technologies for Catalysis in Water

08/15/09-07/31/12

\$600,810

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

A nanomicelle-forming amphiphile "PTS" has been identified that allows for several Pd- and Ru-catalyzed cross-couplings to take place in water as the only solvent, and at room temperature, in high isolated yields. The new processes include Heck, Suzuki, Sonogashira, and olefin cross-metathesis reactions, where product isolation is especially facile. Several additional studies are planned based on the "micellar effect." The notion of "designer" surfactants applied to organometallic catalysis is advanced in this proposal, and represents a variable essentially overlooked by the synthetic community. This technology also is to be applied to other important cross-couplings, such as aminations and asymmetric additions of hydride to Michael acceptors, all in water at room temperature.

Bruce Lipshutz

National Science Foundation, CHE-0937658

EAGER: Chemistry of Water-Intolerant Intermediates....in Water

09/01/09-08/31/12

\$200,000

This award is funded under the American Recovery and Reinvestment Act of 2009 (Public Law 111-5).

This project will initiate work on the development of methods for two unprecedented reactions: (1) in situ Grignard formation and use in cross-coupling reactions in water, and (2) formation of unstabilized

ylides for Wittig-like olefinations, also in water. These will take advantage of micellar catalysis, where the reactive species to be generated either on the surface of the metal, or within a micelle, are protected from their aqueous surroundings by the hydrophobic interior of these nanoparticles. For these studies, many variables will need to be screened, including the nature of the amphiphile that is to supply a dry reaction medium, in water.

With this award, the Organic and Macromolecular Chemistry Program is supporting the research of Professor Bruce H. Lipshutz of the Department of Chemistry at the University of California, Santa Barbara. Professor Bruce Lipshutz's research efforts revolve around the development of new synthetic methods for the formation of C-C, C-H, C-O, and C-N bonds. Such chemistry will contribute to environmentally benign methods for chemical synthesis, as these new processes will be developed in the absence of organic solvents. Successful development of the methodology will have an impact on synthesis in the pharmaceutical, fine chemicals, and agricultural industries.

Bruce Lipshutz

National Science Foundation, CHE-094879

New Technologies Based on Organocopper Catalysis

06/01/10-05/31/13

\$489,000

This project will explore several synthetic methods that rely on copper as the metal that effects catalysis. A number of the transformations are on copper hydride chemistry, which includes new uses of nonracemically ligated CuH for syntheses. The potential to realize unprecedented ligand-accelerated catalysis with CuH in pure water at room temperature will be pursued, along with the potential to deliver water-sensitive carbon-based residues via conjugate addition chemistry, with both approaches based on micellar catalysis in water. Heterogeneous processes that take advantage of both readily accessed valence states of copper [Cu(I) and Cu(II)] impregnated into the pores of inexpensive charcoal matrices will also be developed. A high substrate-to-ligand ratio and tandem processes that can be carried out in a single reaction vessel will be studied.

With this award, the Chemical Synthesis Program is supporting the research of Professor Bruce H. Lipshutz of the Department of Chemistry at the University of California, Santa Barbara. Professor Lipshutz's research efforts revolve around the development of organocopper-based asymmetric catalysis leading to new methods for the formation of C-C and C-H bonds. Such chemistry will contribute to environmentally benign methods for chemical synthesis as most of these new technologies will be developed in the absence of organic solvents, where water serves as the macroscopic medium. Successful applications of the methodology will have an impact on synthesis in the pharmaceutical, fine chemical, and agricultural industries.

Philip Lubin

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NOTE: Dates in **red** are the projected end dates and dollar value in **red** is the projected total award value.

Jet Propulsion Laboratory, JPL1367008
Planck Educational and Public Outreach Effort at UCSB
02/10/09-09/30/13
\$45,700 (~~\$67,000~~)

This award will fund a cosmology summer session that brings in students from a local high school (Dos Pueblos High and perhaps others) and a local community college (Santa Barbara City College). Graduate students, post doc (Rodrigo) Peter Meinhold and Dr. Lubin will orient the students on the Planck mission and relevant science and technology issues, and then the students will work during the summer as a team on various CMB technology programs for a hands-on summer program. We hope to run this program over a six week period each summer.

Douglas Scalapino
Oak Ridge National Laboratory, 4000068439
Studies of the Properties of Strongly Correlated Materials
04/14/08-03/31/12
\$403,301 (~~\$446,886~~)

Using recently developed algorithms and new state of the art computer hardware and architecture, we are seeking to understand the properties of strongly correlated electronic materials. Our work is particularly focused on the challenges posed by the high temperature cuprate superconductors. We believe that an understanding of these materials will open an important area of material science and applications.

Mark Sherwin
S. James Allen
Elliott Brown
Song-I Han
Philip Lubin
Kevin Plaxco
Mark Rodwell
William M. Keck Foundation, SB080017
“Filming” Proteins in Action with UC Santa Barbara’s Free Electron Lasers
07/01/07-06/30/11
\$1,750,000

The movement and dynamics of proteins is of enormous importance in almost all of the biological processes and reactions that occur in living organisms. Unfortunately, however, our ability to characterize these motions is limited by the fact that proteins perform their biological roles in aqueous solution, a milieu that poses nearly intractable problems for established experimental methodologies to study molecular dynamics. Here we propose a research program dedicated to the hitherto difficult task of monitoring the collective, functional motions of proteins and other biomolecules in aqueous solution. The program will receive significant leveraging from UC Santa Barbara's unique existing suite of high power terahertz free electron lasers. We will pioneer the development and application of two complementary techniques by which protein motions *in aqueous solution* can be "filmed:"

1. terahertz absorption spectroscopy of proteins and
2. terahertz pulsed electron paramagnetic resonance.

Taken together the two approaches will provide revolutionary insights into the dynamics of proteins as they function in their biologically relevant environments.

Mark Sherwin

National Science Foundation, DMR-1006603

Quantum Coherence and Dynamical Instability in Quantum Wells Driven by Intense Terahertz Fields

08/15/10-07/31/12 (07/31/14)

\$290,000 (\$560,000)

Beginning when early humans harnessed fire for heat and light, the control of electromagnetic radiation has been central to the development of our species. The notion of electromagnetic radiation is nearly 150 years old, proposed by Maxwell in 1865 and demonstrated with the discovery of radio waves in 1866. Radio waves remained largely a laboratory curiosity for nearly 50 years. It is difficult to imagine modern life without radio waves, microwaves, heat, light, and X-rays, which are now all understood to be manifestations of electromagnetic radiation, listed in order of increasing frequency. However, lying between the frequencies of microwaves and heat, stretching from 0.1 to 10 trillion cycles per second (0.1-10 terahertz) is the so-called 'terahertz gap.' Electromagnetic waves exist in this frequency range, but they are extremely difficult to generate and control. This individual investigator award supports a project that will use the world's brightest pulses of terahertz waves, generated by accelerator-driven 'free-electron lasers', to search for new quantum-mechanical phenomena predicted to occur in nanometers-thick semiconductor devices. The semiconductor devices under study are similar to those used to modulate light in fiber-optic communications, and as ultrafast transistors in cellular telephones. This project will support the education of two PhD students, as well as undergraduate and high-school interns. The students will learn the most advanced techniques to generate and manipulate electromagnetic radiation across the electromagnetic spectrum, preparing them for leadership in the

nation's scientific and technological workforce, and bringing mankind closer to harnessing terahertz radiation for future technologies.

Mark Sherwin

Tanner Research Inc., UCSB FA9550-10-C-0177

Frequency Agile THz Detectors for Multiplicative Mixing

09/30/10-08/31/11

\$35,000

Prototypes fabricated by Tanner will be tested at UCSB using the world's best set of terahertz sources, detectors, and spectroscopy systems. The tests will measure metrics defined in the metrics model. We have in the past measured responsivity, noise and noise-equivalent power for self-mixing detectors at 1 THz. Such measurements can be performed on the multiplicative mixer devices, which can also operate as self mixers. Many of the relevant metrics for multiplicative mixers will be similar to those for additive mixers—for example, noise temperature. We have experience measuring the noise temperatures of additive mixers (Schottky diode superheterodyne receivers) at 240 GHz, and can easily extend these measurements, with equipment on hand, to 700 GHz. We will develop techniques to measure other important metrics, such as mixer conversion gain or loss (ratio of power at the intermediate frequency to THz signal power for heterodyne mixing). The Free-Electron-Lasers will be especially useful for measurements at frequencies above 1 THz. Terahertz time-domain spectrometers (broad-band, 0.1-3 THz) or a vector network analyzer with frequency extenders (phase-sensitive measurements 70-700GHz with up to 120 dB dynamic range).

Jatila van der Veen

Phillip Lubin

Jet Propulsion Laboratory, JPL 1388406

The Planck Visualization Project: Education and Public Outreach Effort of the U.S.

Planck Mission

10/01/09-09/30/13

\$120,800 (~~\$229,049~~)

Planck is a mission to measure the anisotropy of the cosmic microwave background (CMB), sponsored by the European Space Agency (ESA) with significant input from NASA. Launched on May 14, 2009, Planck will measure the sky across nine frequency channels, with temperature sensitivity of 10^{-6} K, and spatial resolution up to 5 arc minutes.

NASA participation in Planck is approved and funded, and is managed by the Planck Project at the Jet Propulsion Laboratory in Pasadena, California. The US Planck project is required by NASA to perform Education and Public Outreach (E/PO) as an integral part of the science development. This award serves at the focal point for the E/PO activities of the US Planck team

Contracts/Grants Awarded 2010-2011

Department of Air Force Office of Scientific Research

Michael Bowers

FA9550-11-1-0113 06/15/2011-06/14/2014 \$ 190,000

Litigated Metal Clusters: Structures, Energetics and Reactivity

Jet Propulsion Laboratory

Philip Lubin

1367008 02/10/09-09/30/13 \$ 10,700

Planck Educational and Public Outreach Effort at UCSB

Philip Lubin

1367008 02/10/09-09/30/13 \$ 5,000

Planck Educational and Public Outreach Effort at UCSB

Jatila van der Veen, Philip Lubin

1388406 10/01/09-09/30/2013 \$ 5,000

The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Plank Mission

Jatila van der Veen, Philip Lubin

1388406 10/01/09-09/30/2013 \$ 28,700

The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Plank Mission

Jatila van der Veen, Philip Lubin

1388406 10/01/09-09/30/2013 \$ 28,700

The Planck Visualization Project: Education and Public Outreach Effort of the U.S. Plank Mission

Jet Propulsion Laboratory Subtotal \$ 78,100

National Science Foundation

Guenter Ahlers

DMR-0702111 05/01/07-04/30/12 \$ 155,000

Turbulent Convection in a Fluid Heater from Below

Dirk Bouwmeester

PHY-0804177 08/01/08-07/31/12 \$ 160,000

Quantum States of OptoMechanical Structures

Mark Sherwin
DMR-1006603 08/15/10-07/31/11 \$ 155,000
Quantum Coherence and Dynamical Instability in Quantum Wells Driven by Intense Terahertz Fields

Mark Sherwin
DMR-1006603 08/15/10-07/31/11 \$ 135,000
Quantum Coherence and Dynamical Instability in Quantum Wells Driven by Intense Terahertz Fields

National Science Foundation Subtotal \$ 605,000

National Institutes for Health

NIH Center for Scientific Review

Bruce Lipshutz
1R01 GM086485-01A1 08/01/10-07/31/12 \$ 295,906
New Technologies for Catalysis in Water

Oak Ridge National Laboratory (Department of Energy GOCO Operated by UT Batelle, LIC.)

Douglas Scalapino
4000068439 04/14/08-03/31/12 \$ 29,055
Study of the Properties of Strongly Correlated Materials

Douglas Scalapino
4000068439 04/14/08-03/31/12 \$ 43,580
Study of the Properties of Strongly Correlated Materials

Oak Ridge National Laboratory Subtotal \$ 72,635

Tanner Research, Inc

Mark Sherwin
UCSB FA9550-10-C-0177 09/30/10-09/30/11 \$ 35,000
Frequency Agile THz Detectors for Multiplicative Mixing

UC Los Angeles

Michael Bowers
SB070075 09/01/06-07/31/12 \$ 258,369
Pathogenic Protein Folding and Human Disease

Research Support Summary (2010-2011)

			% Total
Federal			
Air Force	190,000	15%	12%
Jet Propulsion Laboratory	78,100	6%	5%
National Science Foundation	605,000	49%	39%
National Institutes for Health	295,906	24%	19%
Oak Ridge National Laboratory	72,635	6%	5%
Federal Totals	\$1,241,641	100%	81%
Private			
Tanner Research, Inc.	35,000	100%	2%
Private Totals	\$35,000	100%	2%
State			
University of California, Los Angeles	258,369	100%	17%
State Totals	\$258,369	100%	17%
TOTALS	\$1,535,010		100.00%

Charts and Graphs

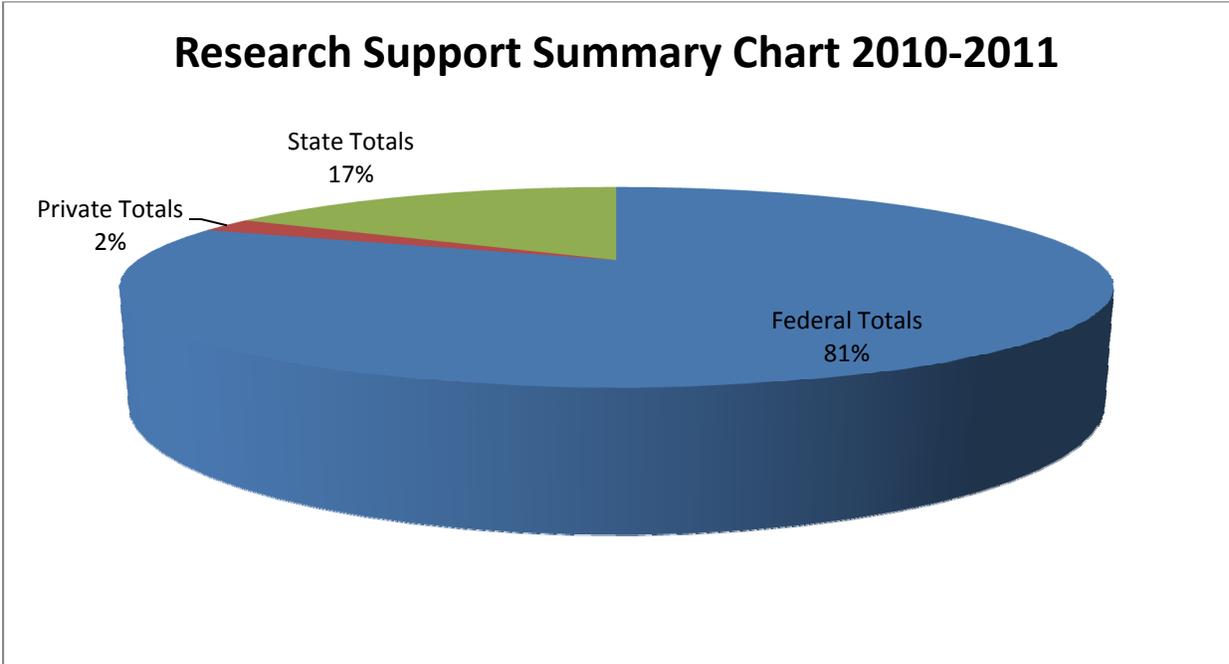


Chart 1: Research Support Summary Chart 2010-2011

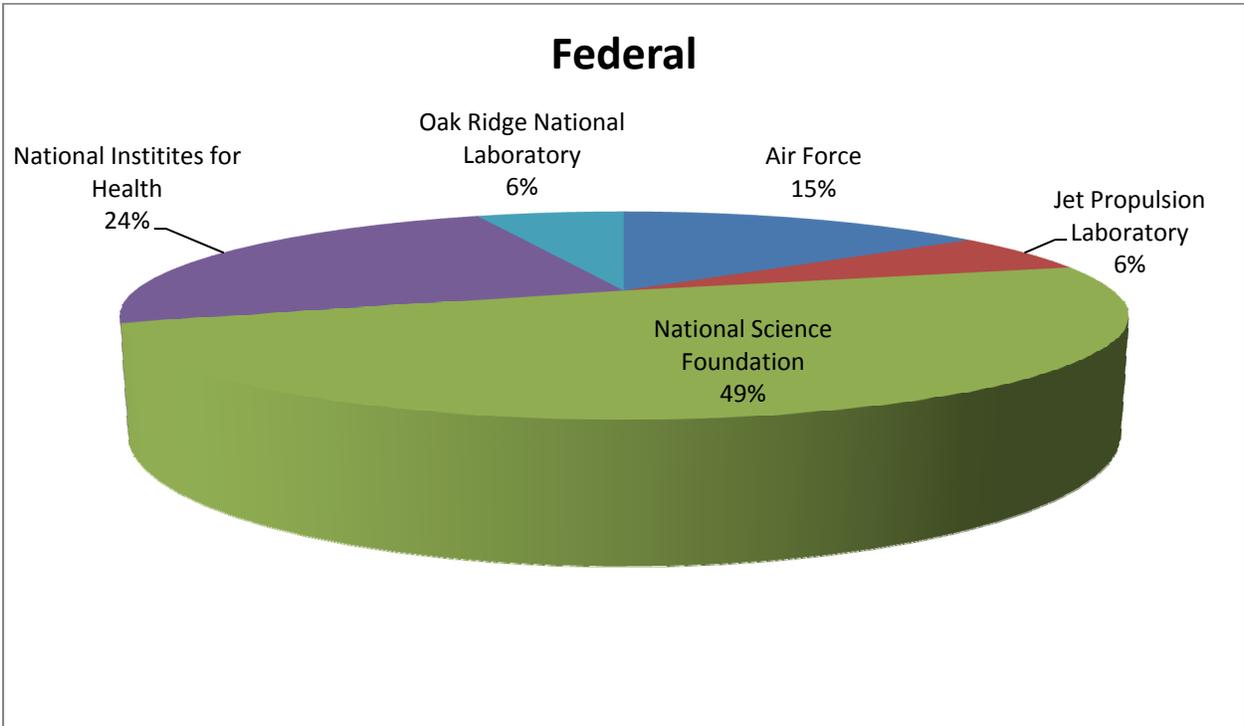
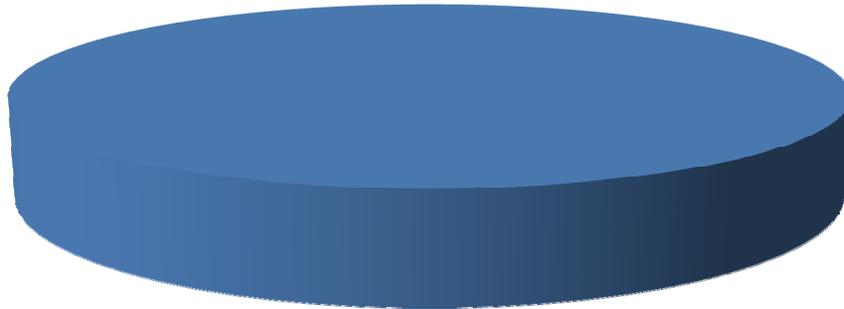


Chart 2: Federal Research Support Summary Chart

State



University of
California, Los
Angeles
100%

Chart 3: State Research Support Summary Chart

Private



Tanner Research, Inc
100%

Chart 4: Private Research Support Summary Chart

Base Budget and Overhead Generated (thousands of dollars)

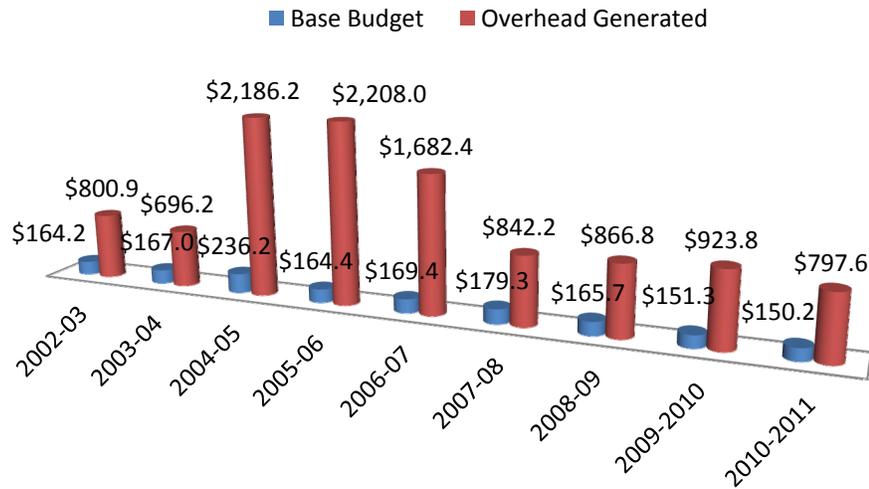


Chart 5: Base Budget and Overhead Generated

Number of Proposals Submitted and Funded

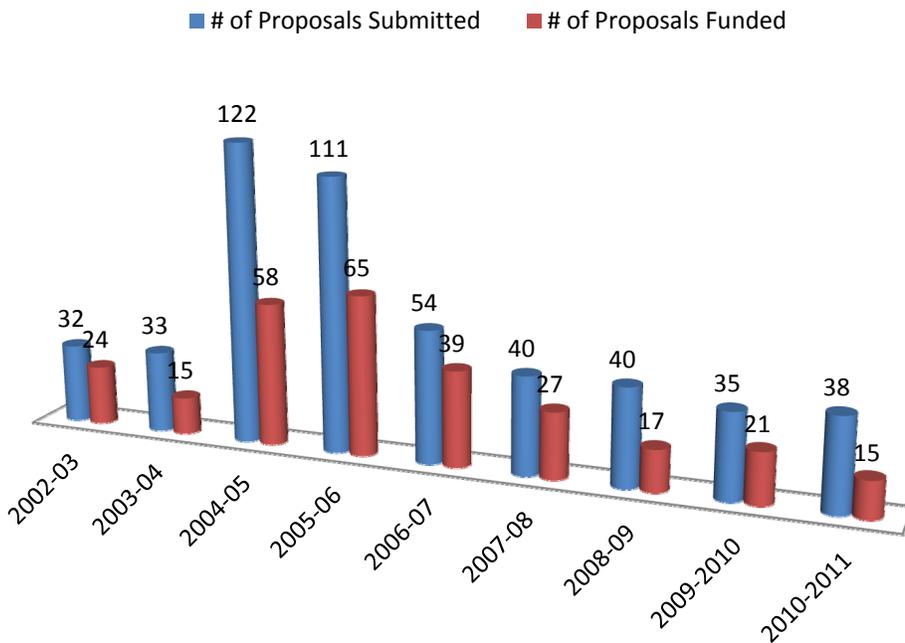


Chart 6: Number of Proposals Submitted and Funded

Value of Proposals Submitted and Funded (millions of dollars)

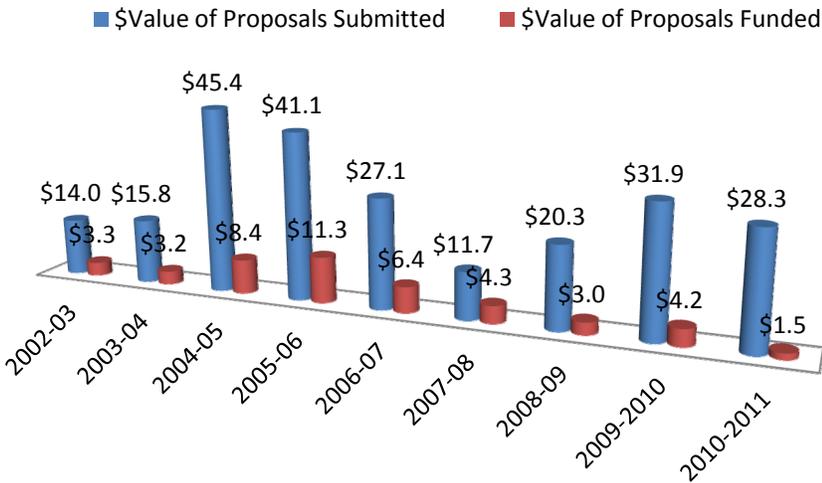


Chart 7: Value of Proposals Submitted and Funded

of Awards Administered

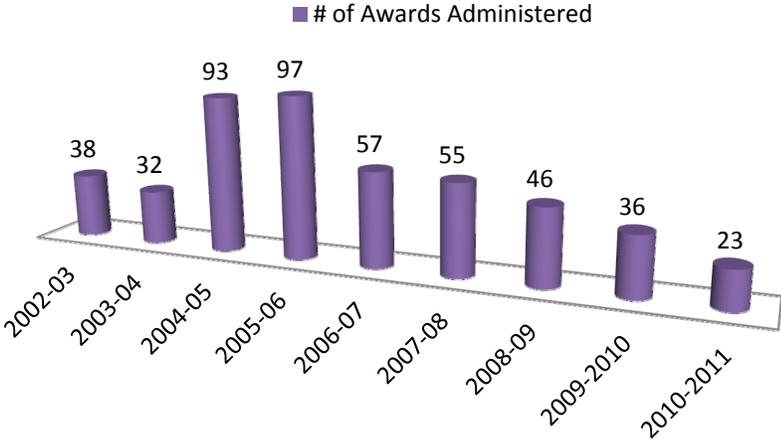


Chart 8: Number of Awards Administered

Value of Contracts and Grants Administered (millions of dollars)



Chart 9: Value of Contracts and Grants Administered

Statistical Summary for ITST

2010-2011

1. Academic personnel engaged in research:	
a. Faculty	25
b. Professional Researchers (including Visiting)	4
c. Project Scientists	10
d. Specialists	12
e. Postdoctoral Scholars	7
f. Postgraduate Researchers	0
TOTAL	58
2. Graduate Students:	
a. Employed on contracts and grants	24
b. Employed on other sources of funds	0
c. Participating through assistantships	0
d. Participating through traineeships	0
e. Other (specify)	0
TOTAL	24
3. Undergraduate Students:	
a. Employed on contracts and grants	10
b. Employed on other funds	0
c. Number of volunteers, & unpaid interns	0
TOTAL	10
4. Participation from outside UCSB: (optional)	
a. Academics (without Salary Academic Visitors)	0
b. Other (City College Student)	1
5. Staff (Univ. & Non-Univ. Funds):	
a. Technical	10
b. Administrative/Clerical	4
6. Seminars, symposia, workshops sponsored	14
7. Proposals submitted	38
8. Number of different awarding agencies dealt with*	15
9. Number of extramural awards administered	23
10. Dollar value of extramural awards administered during year**	\$13,422,416
11. Number of Principal Investigators***	31
12. Dollar value of other project awards ****	\$495,920
13. Number of other projects administered	10
14. Total base budget for the year (as of June 30, 2011)	\$150,158
15. Dollar value of intramural support	\$577,967
16. Total assigned square footage in ORU	7,700
17. Dollar value of awards for year (08 Total)	\$1,535,010
* Count each agency only once (include agencies to which proposals have been submitted).	
** If the award was open during the year, even if for only one month, please include in total.	
*** Number of PIs, Co-PIs and Proposed PIs (count each person only once.)	
**** Other projects - such as donation, presidential awards, fellowships, anything that isn't core budget, extramural, or intramural.	

Principal Investigators

Guenter Ahlers	Research Professor	Physics
S. James Allen	Research Professor	Physics
Dirk Bouwmeester	Professor	Physics
Michael Bowers	Professor	Chemistry and Biochemistry
Elliot Brown	Professor	Electrical and Computer Engineering
Louis Claude Brunel	Project Scientist	Institute for Terahertz Science and Technology
Steven Buratto	Professor	Chemistry and Biochemistry
David Cannell	Professor	Physics
Andrew Cleland	Professor	Physics
Frederick Dahlquist	Professor	Chemistry and Biochemistry
Deborah Fyngenson	Associate Professor	Physics
Elisabeth Gwinn	Professor	Physics
Song-I Han	Assistant Professor	Chemistry and Biochemistry
Michael Liebling	Assistant Professor	Electrical and Computer Engineering
Everett Lipman	Associate Professor	Physics
Bruce Lipshutz	Professor	Chemistry and Biochemistry
Philip Lubin	Professor	Physics
Benjamin Mazin	Assistant Professor	Physics
Peter Meinhold	Associate Researcher	Physics
Horia Metiu	Professor	Chemistry and Biochemistry
Nguyen, Thuc-quyen	Associate Professor	Chemistry and Biochemistry
Chris Palmstrom	Professor	Electrical and Computer Engineering
Pierre Petroff	Professor	Materials
Kevin Plaxco	Professor	Chemistry and Biochemistry
Mark Rodwell	Professor	Electrical and Computer Engineering
Douglas Scalapino	Research Professor	Physics
Joan-Emma Shea	Professor	Chemistry and Biochemistry
Mark Sherwin	Professor	Physics
Kimberly Turner	Professor	Mechanical & Environmental Engineering
Jatila Van Der Veen	Asst Project Scientist	Institute for Terahertz Science and Technology
Johan van Tol	Assoc Scholar Scientist	Florida State University

Map

